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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	CA/CAplus records now contain indexing from 1907 to the present
NEWS 4	DEC 08	INPADOC: Legal Status data reloaded
NEWS 5	SEP 29	DISSABS now available on STN
NEWS 6	OCT 10	PCTFULL: Two new display fields added
NEWS 7	OCT 21	BIOSIS file reloaded and enhanced
NEWS 8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 9	NOV 24	MSDS-CCOHS file reloaded
NEWS 10	DEC 08	CABA reloaded with left truncation
NEWS 11	DEC 08	IMS file names changed
NEWS 12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS 13	DEC 09	STN Entry Date available for display in REGISTRY and CA/CAplus
NEWS 14	DEC 17	DGENE: Two new display fields added
NEWS 15	DEC 18	BIOTECHNO no longer updated
NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS 17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes
NEWS 23	MAR 03	MEDLINE and LMEDLINE reloaded
NEWS 24	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS 25	MAR 03	FRANCEPAT now available on STN

NEWS EXPRESS	MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:59:35 ON 18 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:59:42 ON 18 MAR 2004
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAR 2004 HIGHEST RN 664302-53-8
DICTIONARY FILE UPDATES: 17 MAR 2004 HIGHEST RN 664302-53-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\09759633.str

L1 STRUCTURE UPLOADED

=> s l1 ful
FULL SEARCH INITIATED 12:00:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 407 TO ITERATE

100.0% PROCESSED 407 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

L2 25 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 12:00:12 ON 18 MAR 2004

FILE COVERS 1907 - 18 Mar 2004 VOL 140 ISS 12
FILE LAST UPDATED: 17 Mar 2004 (20040317/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

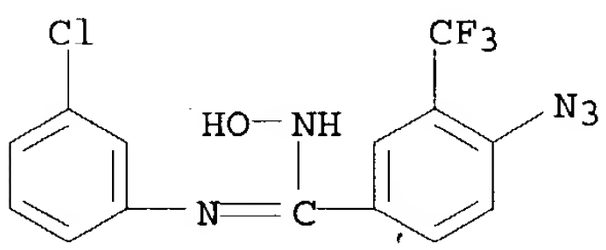
=> s l2
L3 10 L2

=> d l3 ibib hitstr abs 1-10

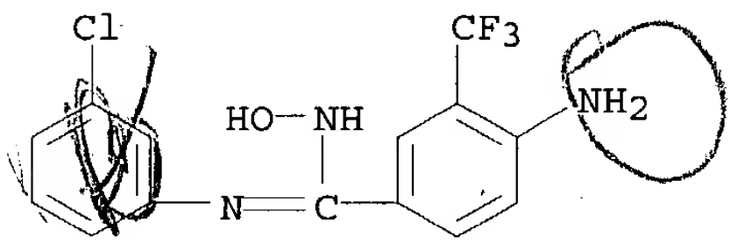
L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:526050 CAPLUS
DOCUMENT NUMBER: 135:107149
TITLE: Synthesis, antibacterial activity and RNA polymerase inhibition of phenylamidine derivs.
INVENTOR(S): Li, Leping; Chen, Xiaoqui; Fan, Pingchen; Mihalic, Jeffrey Thomas; Cutler, Serena
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001051456	A2	20010719	WO 2001-US1219	20010112
WO 2001051456	A3	20011220		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002045749	A1	20020418	US 2001-759633	20010112
EP 1246795	A2	20021009	EP 2001-914329	20010112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

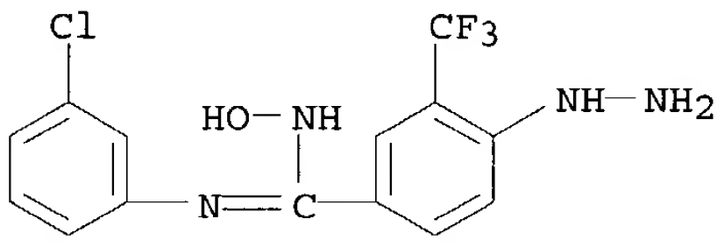
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2003519676 T2 20030624 JP 2001-551838 20010112
PRIORITY APPLN. INFO.: US 2000-175892P P 20000113
WO 2001-US1219 W 20010112
OTHER SOURCE(S): MARPAT 135:107149
IT **350486-82-7P 350486-84-9P 350486-86-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis, antibacterial activity and RNA polymerase inhibition of phenyl- and heterocyclylhydroxyamidine derivs.)
RN 350486-82-7 CAPLUS
CN Benzenecarboximidamide, 4-azido-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350486-84-9 CAPLUS
CN Benzenecarboximidamide, 4-amino-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



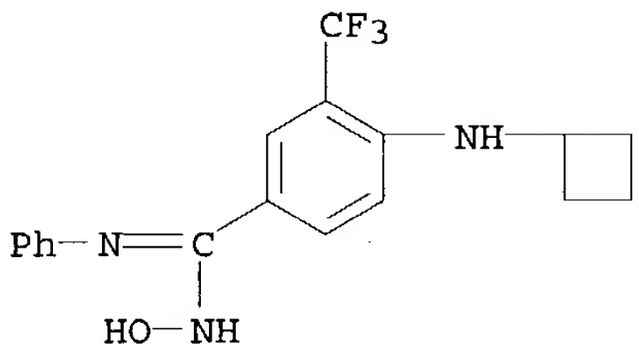
RN 350486-86-1 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-hydrazino-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



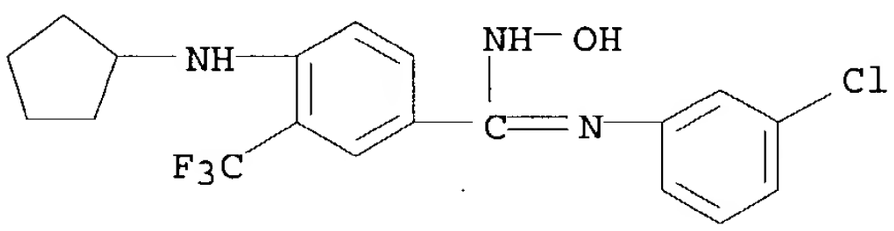
IT **350487-08-0P 350487-09-1P 350487-13-7P**
350487-14-8P 350487-15-9P 350487-18-2P
350487-19-3P 350487-20-6P 350487-22-8P
350487-25-1P 350487-26-2P 350487-31-9P
350487-96-6P 350487-97-7P 350487-98-8P
350487-99-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis, antibacterial activity and RNA polymerase inhibition of phenyl- and heterocyclylhydroxyamidine derivs.)

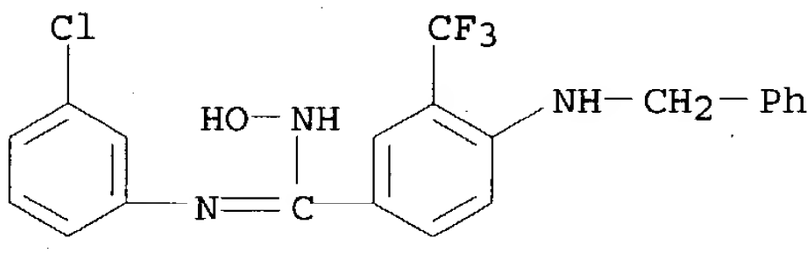
RN 350487-08-0 CAPLUS
CN Benzenecarboximidamide, 4-(cyclobutylamino)-N-hydroxy-N'-phenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



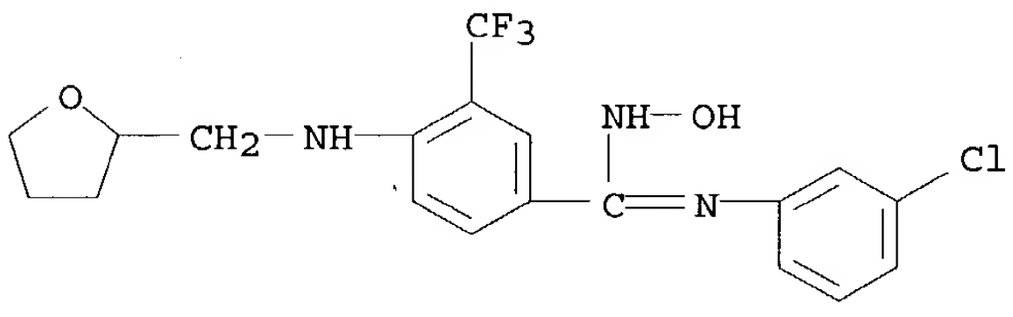
RN 350487-09-1 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-(cyclopentylamino)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-13-7 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(phenylmethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

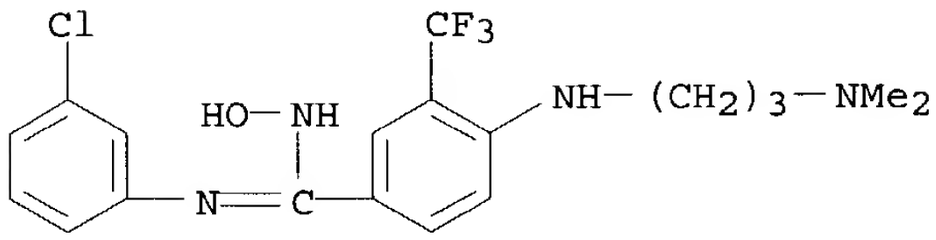


RN 350487-14-8 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[[(tetrahydro-2-furanyl)methyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

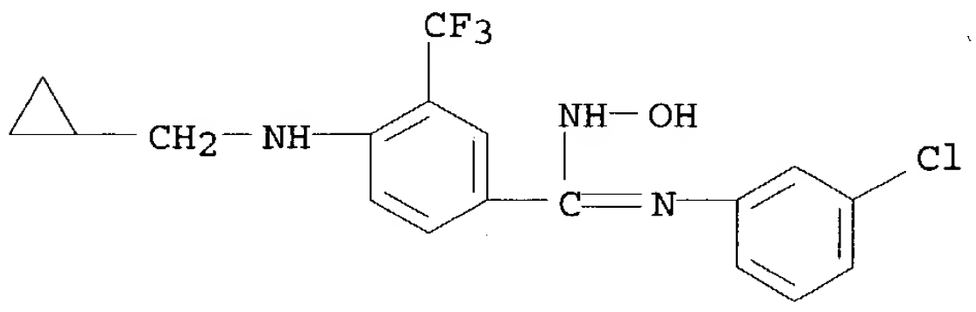


RN 350487-15-9 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-[[3-

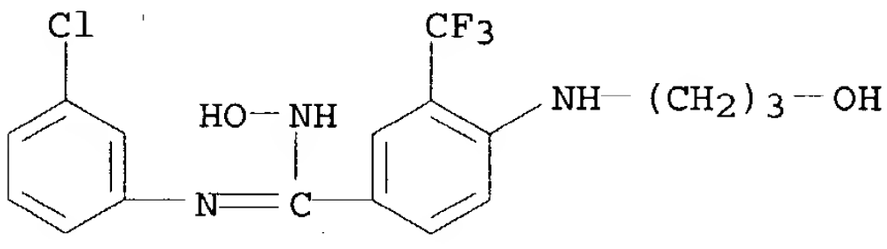
(dimethylamino)propyl]amino]-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



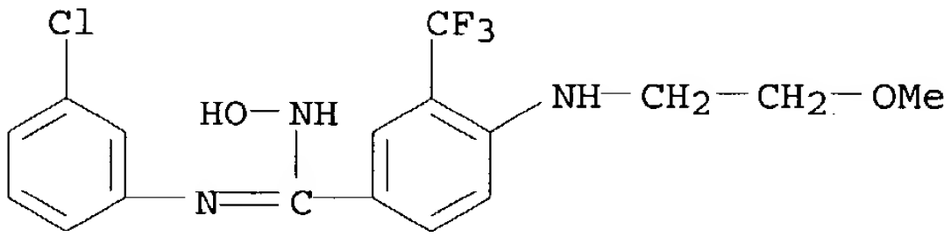
RN 350487-18-2 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-[(cyclopropylmethyl)amino]-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



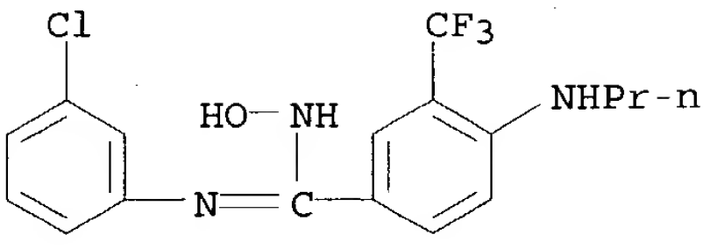
RN 350487-19-3 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(3-hydroxypropyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



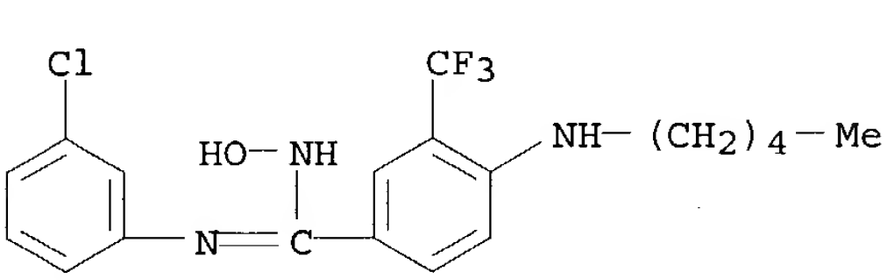
RN 350487-20-6 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(2-methoxyethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



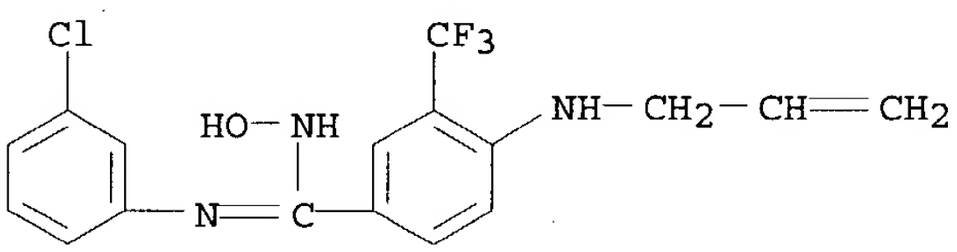
RN 350487-22-8 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(propylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



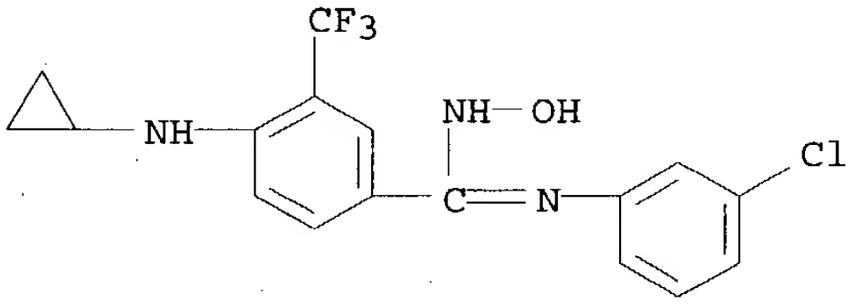
RN 350487-25-1 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(pentylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



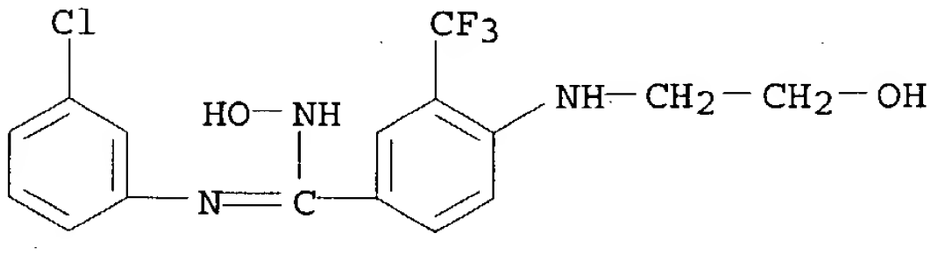
RN 350487-26-2 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(2-propenylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



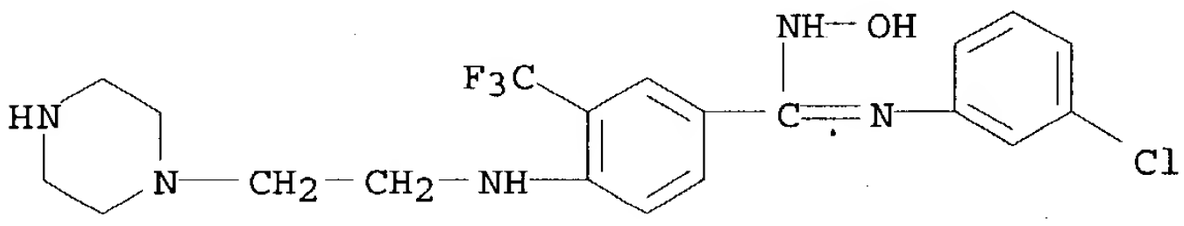
RN 350487-31-9 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-(cyclopropylamino)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



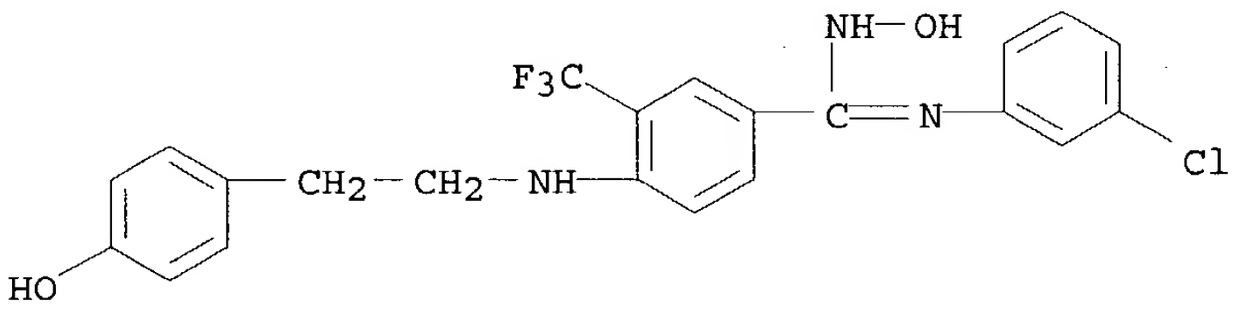
RN 350487-96-6 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(2-hydroxyethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



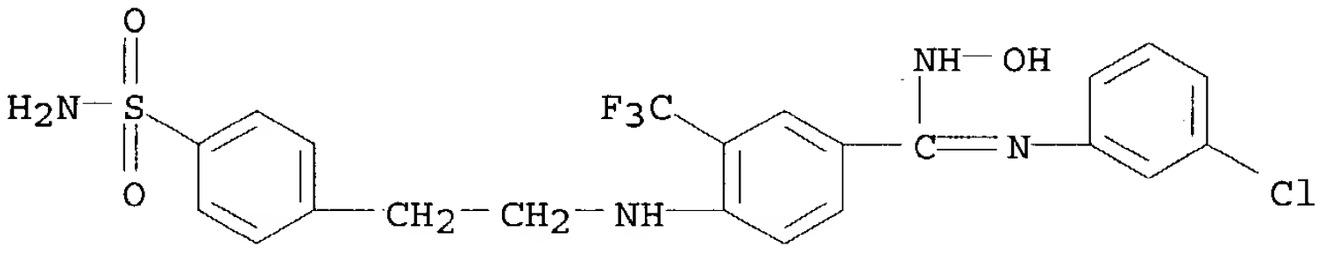
RN 350487-97-7 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[[2-(1-piperazinyl)ethyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



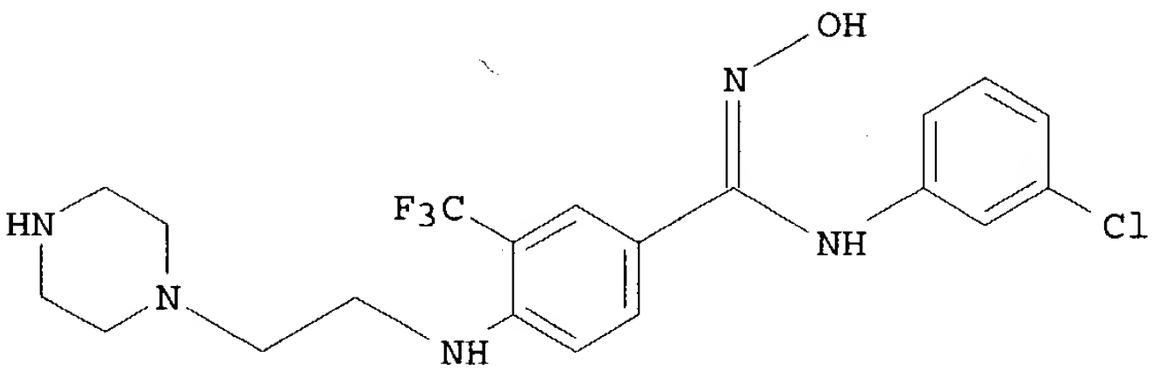
RN 350487-98-8 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[[2-(4-hydroxyphenyl)ethyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-99-9 CAPLUS
CN Benzenecarboximidamide, 4-[[2-[4-(aminosulfonyl)phenyl]ethyl]amino]-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



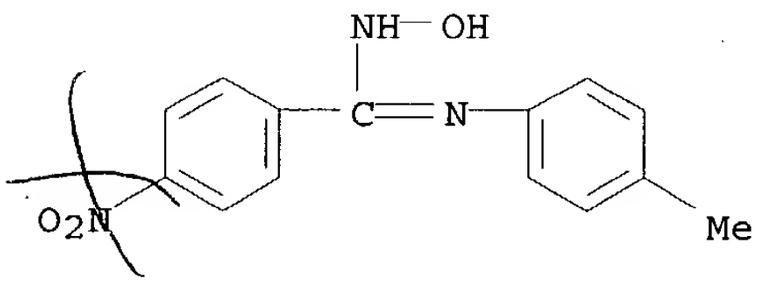
GI



I

AB Synthesis of hydroxyamidines, e.g. (I) and related compds. are disclosed which are suitable as antibacterial agents by their inhibition of RNA polymerase. Antibacterial activity against S. aureus and E. coli are given.

L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:276393 CAPLUS
DOCUMENT NUMBER: 133:73985
TITLE: A convenient synthesis of 3,4-disubstituted-1,2,4-thiadiazole-5(4H)-thiones
AUTHOR(S): Agirbas, Hikmet; Kahraman, Kazim
CORPORATE SOURCE: Department of Chemistry, Kocaeli University, Izmit, 41300, Turk.
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1998), 134/135, 381-389
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **2630-07-1**, N-Hydroxy-N'-(4-methylphenyl)-4-nitrobenzenecarboximidamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiadiazolethiones by rearrangement of oxadiazolethione intermediates)
RN 2630-07-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-N'-(4-methylphenyl)-4-nitro- (9CI) (CA INDEX NAME)

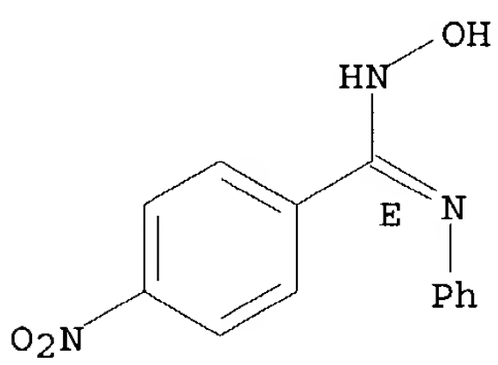


AB 3,4-Disubstituted-1,2,4-oxadiazole-5(4H)-ones were obtained from the reaction of substituted amide oximes with Et chloroformate. These compds. were treated with P2S5 to give corresponding 1,2,4-oxadiazole-5-thiones. Rearrangement of 1,2,4-oxadiazole-5-thiones, catalyzed by metallic copper, yielded 1,2,4-thiadiazole-5-ones. The reaction of 1,2,4-thiadiazole-5-ones with P2S5 gave 1,2,4-thiadiazole-5-thiones.
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:908286 CAPLUS
DOCUMENT NUMBER: 124:102365
TITLE: Crystal and molecular structure of N-phenyl-4-nitrobenzamidoxime
AUTHOR(S): Buzykin, B. I.; Dokuchaev, A. S.; Kharitonova, O. A.
CORPORATE SOURCE: A. E. Arbuzov Inst. Org. Phys. Chem., Russian Acad. Sci., Kazan, 420083, Russia
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1995), (8), 1516-19
CODEN: IASKEA
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **172540-77-1**
RL: PRP (Properties)
(crystal structure of)
RN 172540-77-1 CAPLUS

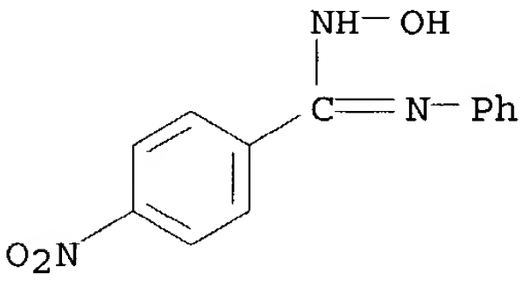
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



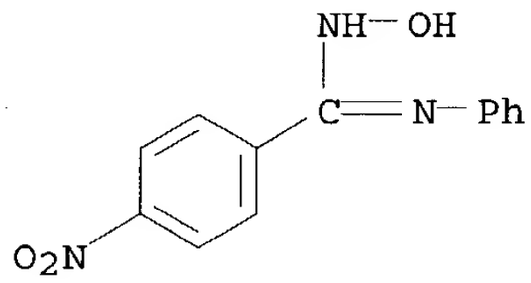
AB An x-ray study of N-phenyl-4-nitrobenzamidoxime (1) was performed. Crystallog. data and atomic coordinates are given. Two crystallog. independent mols. have a planar Z-configuration of amidoxime with s-trans-conformation of these fragments related to =N-O and C-N(H) bonds. Intramol. NH...O bond is observed Rotation angle of nitrophenyl and Ph rings related to amidoxime plane [ONCN] is -57 and -32° in 1A and -38 and -22° in 1B correspondingly. Rotation around C(1)-N(2) bond is -28 (1A) and -35° (1B). 1A and 1B mols. form oxime dimers in crystals due to two intermol. H-bond =N...(HO)', dimers forming double chains due to two more H-bonds NH...(O2N).

L3 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:128321 CAPLUS
DOCUMENT NUMBER: 116:128321
TITLE: Reaction of triethyl orthoformate with mono-substituted amidoximes
AUTHOR(S): Andrianov, V. G.; Eremeev, A. V.
CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1991), 27(8), 1604-7
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **57767-04-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with tri-Et orthoformate)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)

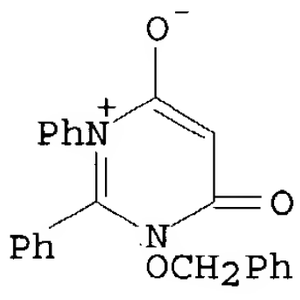


AB The reaction of 4-O2NC6H4C(:NOH)NHR (I; R = Me, Et, Ph) with CH(OEt)3 gave 4-O2NC6H4C(:NO2CNHR)NHR in 33-38% yield. I in turn were prepared from 4-O2NC6H4CCl:NOH and RNH2.

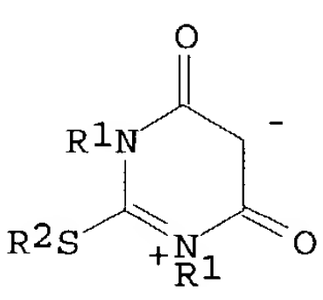
L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:62359 CAPLUS
DOCUMENT NUMBER: 88:62359
TITLE: Syntheses of heterocycles, CCVII. Mesoionic pyrimidines and thiazines
AUTHOR(S): Ziegler, Erich; Steiger, Wilfried; Strangas, Charilaos
CORPORATE SOURCE: Inst. Org. Chem., Univ. Graz, Graz, Austria
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1977), 32B(10), 1204-8
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: German
IT **57767-04-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbon suboxide)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



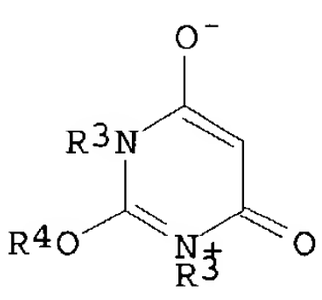
GI



I



II

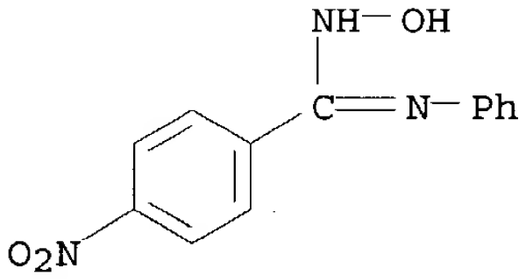


III

AB CH2(CO2N:CRNHPh)2 (R = 4-O2NC6H4, 3-O2NC6H4, 2-ClC6H4) were obtained by treating HON:CRNHPh with C3O2. PhCH2ON:CPhNHPh similarly gave the pyrimidinone I. II (R1 = Ph, 4-MeC6H4, 2-MeC6H4; R2 = Me, Et) were similarly obtained from R1N:C(SR2)NHR1 and III (R3 = cyclohexyl, Ph, 4-MeC6H4, R4 = Me, Et) from R3NHC(OR4):NR3.

L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:542212 CAPLUS
DOCUMENT NUMBER: 85:142212
TITLE: Elimination reactions with anilide oxime o-chlorobenzoates: rearrangement into carbodiimides by reaction with sodium tert-amylate
AUTHOR(S): Garapon, Jacques; Sillion, Bernard
CORPORATE SOURCE: Inst. Fr. Pet., CEN, Grenoble, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1975), (11-12, Pt. 2), 2671-6
CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 85:142212
IT **57767-04-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



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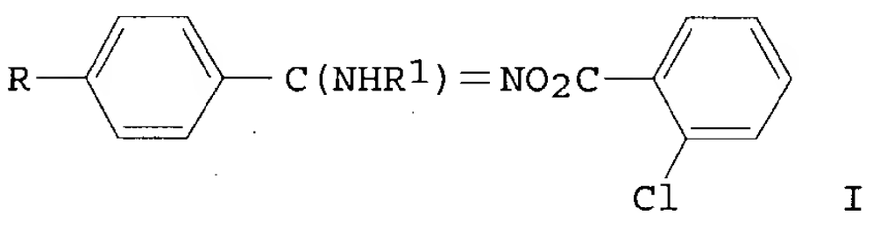
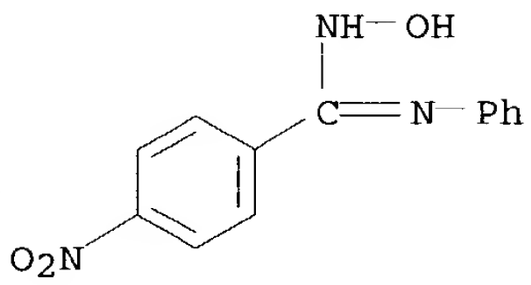


I

AB The elimination reaction of I (R = H, p-MeO, p-NO2; R1 = Ph, cyclohexyl, 2,6-Me2C6H3) with sodium tert-amylate occurred via a carbodiimide intermediate. A concerted reaction mechanism was postulated.

L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:592705 CAPLUS
DOCUMENT NUMBER: 83:192705
TITLE: Synthetic reactions using transition metal complexes. Conversion of amide oximes into amidines by pentacarbonyliron and evidence for imine intermediates in the deoximation of ketoximes
AUTHOR(S): Dondoni, Alessandro; Barbaro, Gaetano
CORPORATE SOURCE: Ist. Chim. Org., Univ. Bologna, Bologna, Italy
SOURCE: Journal of the Chemical Society, Chemical Communications (1975), (18), 761-2
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 83:192705
IT **57767-04-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive dehydroxylation of, by pentacarbonyliron)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)

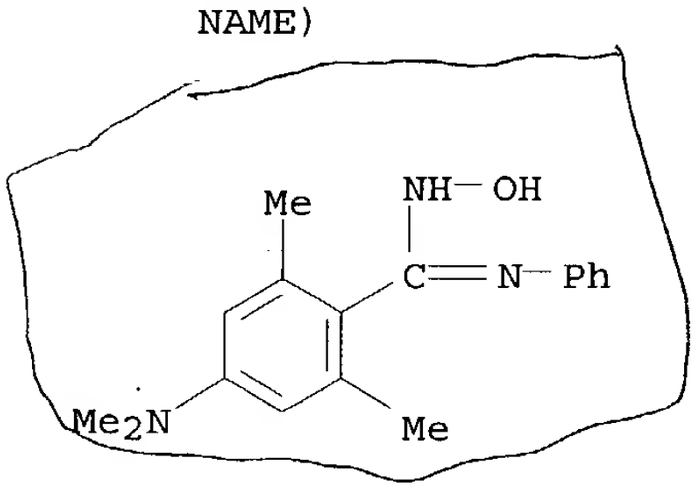


AB Treatment of RC(:NOH)NR1R2 (R = Ph, R1 = H, R2 = Ph, C6H4Cl-p; R = Ph, R1 = Me, R2 = Ph, Me; R = Mesityl, p-O2NC6H4, R1 = H, R2 = Ph) with ≥1 equiv Fe(CO)5 in refluxing dry THF gave 70-90% RC(:NH)NR1R2. 2,4,6-Me3C6H2C(:NOH)Me reacted similarly.

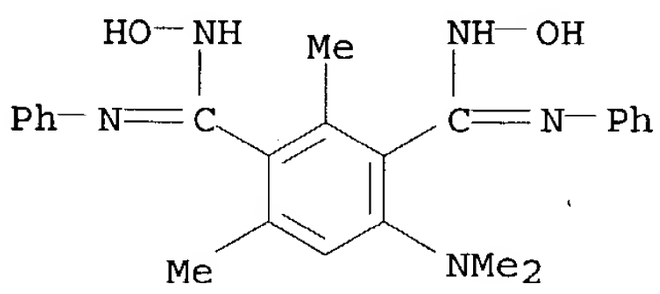
L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:454096 CAPLUS
DOCUMENT NUMBER: 67:54096
TITLE: Nitrile oxides. IX. Basic substituted stable nitrile oxides
AUTHOR(S): Grundmann, Christoph; Richter, Reinhard
CORPORATE SOURCE: Mellon Inst., Pittsburgh, PA, USA
SOURCE: Journal of Organic Chemistry (1967), 32(7), 2308-12
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:54096

IT **13012-21-0P 13012-22-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13012-21-0 CAPLUS
CN Benzamidoxime, 4-(dimethylamino)-2,6-dimethyl-N-phenyl- (8CI) (CA INDEX NAME)



RN 13012-22-1 CAPLUS
CN Isophthalamidoxime, 4-(dimethylamino)-2,6-dimethyl-N,N'-diphenyl- (8CI) (CA INDEX NAME)

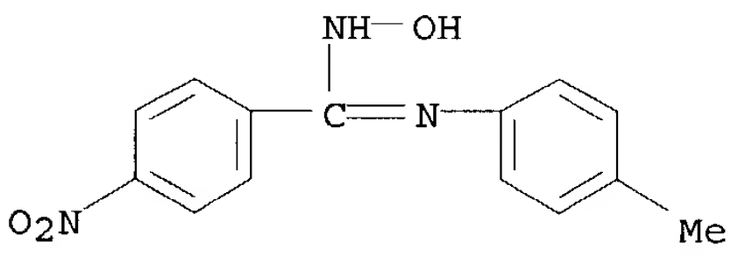


AB cf. CA 66: 37812e. Nitrile oxides of the benzene and pyrimidine series, stabilized by controlled steric hindrance and substituted by a Me2N group,

are described and some of their reactions discussed. These compds. are the 1st isolated nitrile oxides which contain an addnl. different functional group. 21 references.

L3 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1965:431660 CAPLUS
DOCUMENT NUMBER: 63:31660
ORIGINAL REFERENCE NO.: 63:5630f-h,5631a-b
TITLE: Synthesis of 2-oxo-1,2,3,5-oxathiadiazoles
AUTHOR(S): Eloy, F.; Lenaers, R.
CORPORATE SOURCE: Union Carbide European Res. Assoc., Brussels
SOURCE: Bulletin des Societes Chimiques Belges (1965), 74(3-4), 129-35
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French

IT **2630-07-1**, p-Benzotoluidide, 4-nitro-, oxime
(preparation of)
RN 2630-07-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-N'-(4-methylphenyl)-4-nitro- (9CI) (CA INDEX NAME)

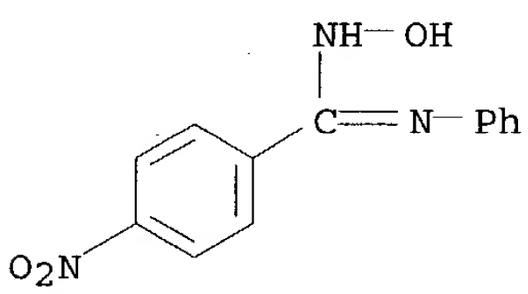


GI For diagram(s), see printed CA Issue.

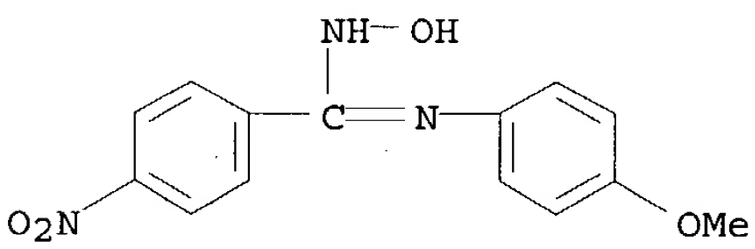
AB A series of derivs. (I) of 2-oxo-1,2,3,5-oxathiadiazole was prepared by the dipolar addition of sulfinylamines to nitrile oxides. I were also formed by treating the appropriate N-substituted amide oxime with SOCl2 in C5H5N. p-C6H4(CNO)2 (3.2 g.) in 100 cc. dioxane stirred .apprx.12 hrs. with 5.6 g. PhNSO (II) yielded 7.6 g. III, m. 180° (decomposition). p-O2NC6H4CCl:NOH (IV) (10 g.) in the min. amount EtOH treated dropwise at -10 to -5° with 6 g. Et3N gave 7.8 g. p-O2NC6H4CNO (V), m. 95°. V (3.3 g.) and 2.8 g. II added at 10° to 100 cc. dry C6H6 and the mixture kept 2 hrs. at room temperature and refluxed 0.5 hr. yielded 6 g. I (R = p-O2NC6H4, R1 = Ph) (VI), m. 140° (C6H6-hexane). IV (10 g.) and 6.9 g. II in 150 cc. dry C6H6 treated with 5 g. Et3N and kept at room temperature overnight gave 4 g. VI, m. 140°. V (1.64 g.) in 50 cc. dry C6H6 treated dropwise with 1.19 g. BuNSO in C6H6 and kept overnight yielded 0.250 g. I (R = p-O2NC6H4, R1 = Bu), m. 54° (petr. ether). IV (20 g.) in 100 cc. dry Et2O treated with 21.4 g. p-MeC6H4NH2 in Et2O and the mixture kept overnight gave 15.5 g. p-O2NC6H4C(:NOH)NHC6H4Me-p (VII), m. 186° (aqueous EtOH). VII (7.8 g.) in 100 cc. dry C6H6 containing 6 cc. C5H5N treated dropwise at 10° with 3.4 g. SOCl2 and the mixture kept 2 hrs. and heated 1 hr. at 80° gave 9.5 g. I (R = p-O2NC6H4, R1 = p-MeC6H4), m. 120° (C6H6-hexane). PrNO2 (26.7 g.) in 1500 cc. dry C6H6, 72 g. PhNCO, and 42 g. II treated dropwise at 15° with 3 cc. Et3N in 20 cc. dry C6H6 and the mixture kept 3 hrs. at room temperature, heated 3 hrs. at 70°, and refrigerated overnight gave 35 g. I (R = Et, R1 = Ph), m. 78° (hexane). Similarly were prepared I (R = Et, R1 = p-MeC6H4), I (R = Et, R1 = p-ClC6H4), and I (R = Et, R1 = p-MeOC6II4) as oils which could not be

obtained pure.

L3 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:38478 CAPLUS
DOCUMENT NUMBER: 56:38478
ORIGINAL REFERENCE NO.: 56:7304c-h
TITLE: Decarboxylation of 1,2,4-oxadiazol-5-ones. Syntheses of benzimidazoles. II
AUTHOR(S): Bacchetti, Tullio; Alemagna, Andreina
CORPORATE SOURCE: Univ. Milan
SOURCE: Atti Accad. Nazl. Lincei, Rend., Classe Sci. Fis., Mat. e Nat. (1960), 28, 824-35
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **57767-04-1**, Benzanilide, 4-nitro-, oxime **96633-78-2**, p-Benzanisidide, 4-nitro-, oxime
(preparation of)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



RN 96633-78-2 CAPLUS
CN p-Benzanisidide, 4-nitro-, oxime (7CI) (CA INDEX NAME)



AB cf. CA 52, 15511g; 55, 16527a. Substituted benzanilide oximes, ArC(:NOH)NHAr', were prepared in 4 ways (A: ArCSNHAr' + NH2OH; B: ArCN → O + Ar'NH2; C: ArCCl:NOH + Ar'NH2; D: ArCCl:NAr' + NH2OH) and converted with ClCO2Et to oxadiazolones. These were decarboxylated by pyrolysis to give in most cases the corresponding benzimidazoles. The following oximes, oxadiazolones, and benzimidazoles were prepared (Ar and Ar', method of preparation, % yield and m.p. of the benzanilide oxime, % yield and m.p. of the corresponding 1,2,4-oxadiazol-5-one, temperature of pyrolysis, and the % yield, name, and m.p. of the product given): Ph, o-MeC6H4, D, -, -, 86, 148°, 220°, 91.5, 2-phenyl-4methylbenzimidazole (246°); Ph, o-O2NC6H4, D, -, -, 86, 125°, 255°, 78, 2-phenyl-4-nitrobenzimidazole (I), -; Ph, m-O2NC6H4, D, 60, 127°, 80, 142°, 190°, 93, I, 194° (40%) [and 2-phenyl-5-nitrobenzimidazole (II), m. 203° (60%)]; Ph, p-O2NC6H4, D, -, 152°, 85, 125°, 230°, 75, II, 203°; p-O2NC6H4, Ph, D, 65, 183°, 90, 201°, 220°, 73.5,

2-(p-nitrophenyl)benzimidazole, 310°; p-MeOC6H4, Ph, D, 45, 120-1°, 90, 160°, 190°, 14, 2-(p-methoxyphenyl)benzimidazole. 227°; p-MeOC6H4, m-O2NC6H4. D, -, 135°, 75, 173°, 190°, 28, 2-(p-methoxyphenyl)-4(and 5)-nitrobenzimidazole, 228-33°; Ph, β-naphthyl, D, 80, 182°, 91, 181°, 220°, 71, 2-phenyl-α(or β)-naphthimidazole (III), -. Ph, α-naphthyl, B, 90, 177°, 89, 141°, 250°, 26.5, III, -. p-O2NC6H4, p-MeOC6H4, D, 70, 163°, 88, 172°, 220°, -, -, -; Ph, p-EtOC6H4, B, 65, 157°, 88, 138°, 250°, -, -, -; Ph, β-pyridyl, A, -, 188°, 50, 168°, 180°, -, -, -.

Two bis(oxadiazolones) were obtained. Oxanilide dioxime refluxed 12 hrs. in dioxane (IV) with ClCO2Et, the precipitate washed with H2O and crystallized from IV yielded 3,3'-bis(4-phenyl-1,2,4-oxadiazol-5-one), m. 265°. Preparation by method C gave 71% oxalo-p-toluidide dioxime (V), m. 201°. V treated in IV with ClCO2Et gave 68% 3,3'-bis(4-p-tolyl-1,2,4-oxadiazol-5-one) m. 261°. Benzanilide oxime (VI) rearranged with PCl5 in Et2O to PhNHCONHPh. Pyrolysis of VI at 165-200° yielded a small amount of 2-phenylbenzimidazole.

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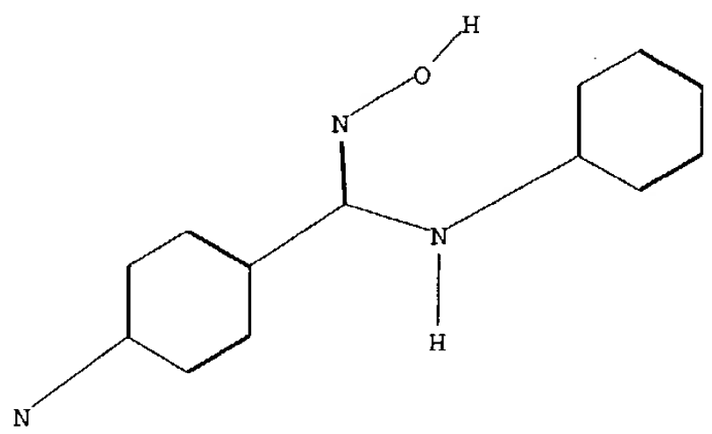

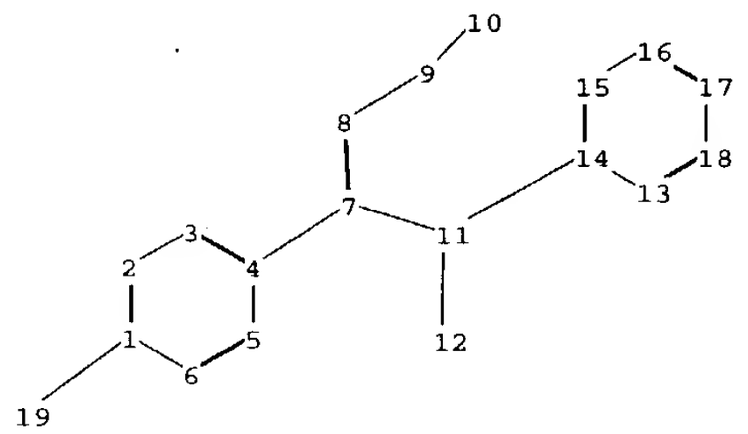

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ring nodes :
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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
1-19 7-8 7-11 8-9 11-14
exact bonds :
4-7 9-10 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 13 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS